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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS	4	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS	5	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS	6	FEB 10	COMPENDEX reloaded and enhanced
NEWS	7	FEB 11	WTEXTILES reloaded and enhanced
NEWS	8	FEB 19	New patent-examiner citations in 300,000 CA/CAPLUS patent records provide insights into related prior art
NEWS	9	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS	10	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS	11	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS	12	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS	13	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS	14	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS	15	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS	16	MAR 11	EPFULL backfile enhanced with additional full-text applications and grants
NEWS	17	MAR 11	ESBIOBASE reloaded and enhanced
NEWS	18	MAR 20	CAS databases on STN enhanced with new super role for nanomaterial substances
NEWS	19	MAR 23	CA/CAPLUS enhanced with more than 250,000 patent equivalents from China
NEWS	20	MAR 30	IMSPATENTS reloaded and enhanced
NEWS	21	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS	22	APR 07	STN is raising the limits on saved answers
NEWS	23	APR 24	CA/CAPLUS now has more comprehensive patent assignee information
NEWS	24	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	25	APR 28	CAS patent authority coverage expanded
NEWS	26	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	27	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS	28	MAY 08	STN Express, Version 8.4, now available
NEWS	29	MAY 11	STN on the Web enhanced

NEWS 30 MAY 11 BEILSTEIN substance information now available on
STN Easy
NEWS 31 MAY 14 DGENE, PCTGEN and USGENE enhanced with increased
limits for exact sequence match searches and
introduction of free HIT display format
NEWS 32 MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal
status data

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 18:00:12 ON 19 MAY 2009

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 18:00:41 ON 19 MAY 2009

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STRUCTURE FILE UPDATES: 18 MAY 2009 HIGHEST RN 1147182-17-9
DICTIONARY FILE UPDATES: 18 MAY 2009 HIGHEST RN 1147182-17-9

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

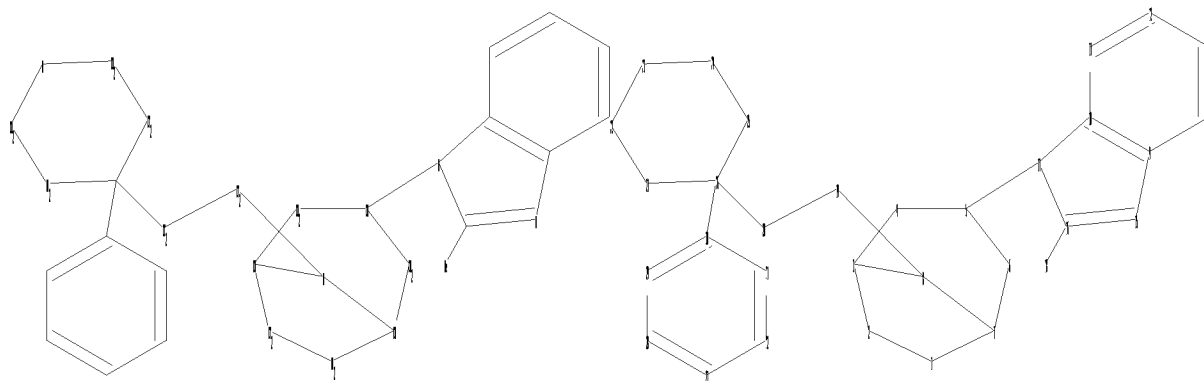
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=>

Uploading C:\Program Files\Stnexp\Queries\10538144genD.str



chain nodes :

18 19 20

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 21 22 23 24 25 26
27 28 29 30 31 32

chain bonds :

5-17 8-19 16-18 19-20 20-26 26-30

ring bonds :

1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 7-8 9-10 9-14 9-15 10-11 10-17 11-12
12-13 13-14 15-16 16-17 21-22 21-26 22-23 23-24 24-25 25-26 27-28 27-32
28-29 29-30 30-31 31-32

exact/norm bonds :

1-2 1-7 2-3 3-4 3-8 4-5 5-6 5-17 6-7 7-8 9-15 10-17 15-16 16-17 21-22
21-26 22-23 23-24 24-25 25-26

exact bonds :

8-19 16-18 19-20 20-26 26-30

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 27-28 27-32 28-29 29-30 30-31 31-32

Match level :

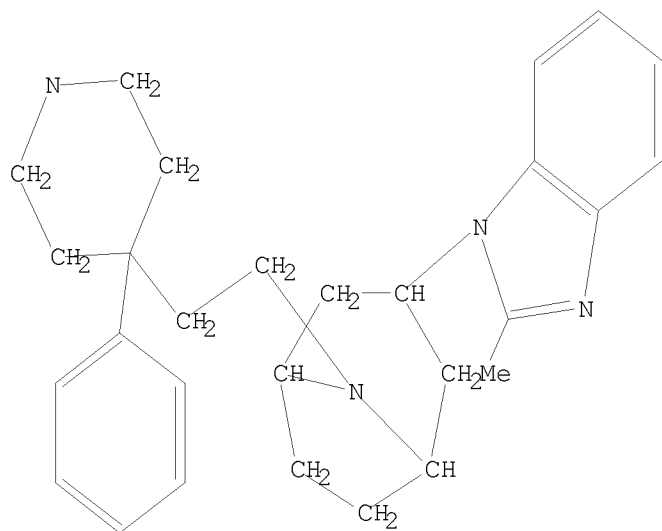
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom
29:Atom 30:Atom 31:Atom 32:Atom

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 18:01:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1294 TO ITERATE

100.0% PROCESSED 1294 ITERATIONS
SEARCH TIME: 00.00.01

1233 ANSWERS

L2 1233 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.36

186.58

FILE 'CAPLUS' ENTERED AT 18:01:46 ON 19 MAY 2009

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FILE COVERS 1907 - 19 May 2009 VOL 150 ISS 21

FILE LAST UPDATED: 18 May 2009 (20090518/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

Caplus now includes complete International Patent Classification (IPC)

reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate

=> s 12

L3 2 L2

=> d 13 abs ibib

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

AB We describe robust chemical approaches toward putative CCR5 scaffolds designed in our labs. Evaluation of analogs in the 125I-[MIP-1 β] binding and Ba-L-HOS antiviral assays resulted in the discovery of 64 and 68 in the 4,4-disubstituted piperidine class H, both potent CCR5 ligands (pIC₅₀ = 8.30 and 9.00, resp.) and HIV-1 inhibitors (pIC₅₀ = 7.80 and 7.84, resp., in Ba-L-HOS assay). In addition, 64 and 68 were bioavailable in rodents, establishing them as lead mols. for further optimization toward CCR5 clin. candidates.

ACCESSION NUMBER: 2008:1154437 CAPLUS

DOCUMENT NUMBER: 149:486141

TITLE: Discovery of Bioavailable 4,4-Disubstituted Piperidines as Potent Ligands of the Chemokine Receptor 5 and Inhibitors of the Human Immunodeficiency Virus-1

AUTHOR(S): Kazmierski, Wieslaw M.; Aquino, Christopher; Chauder, Brian A.; Deanda, Felix; Ferris, Robert; Jones-Hertzog, Deborah K.; Kenakin, Terrence; Koble, Cecilia S.; Watson, Christian; Wheelan, Pat; Yang, Hanbiao; Youngman, Michael

CORPORATE SOURCE: Infectious Diseases Center for Excellence in Drug Discovery, Molecular Discovery Research, Computational and Structural Chemistry, Drug Discovery, IT ID DMPK, Metabolic Pathways Center for Excellence in Drug Discovery, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA

SOURCE: Journal of Medicinal Chemistry (2008), 51(20), 6538-6546

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 13 2 abs ibib

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl, carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl,

heteroarylcycloalkyl, aralkylcarbonyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thioxo groups or halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoimino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocarbonyl, oxyiminomethyl, thioiminomethyl, amino(cyanoimino)methyl, (cyanoimino)methyl, amino(acylimino)methyl, amino(sulfonylimino)methyl, amino(sulfinylimino)methyl, amino(alkoxyimino)methyl, amino(imino)methyl, (cyanoimino)methoxy, iminomethoxy, (cyanoimino)methanethiyl, alkylcarbonyloxy; A = saturated, partially saturated, or aromatic monocyclic

ring

with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5 nitrogen, oxygen, and/or sulfur atoms] such as II are prepared I are prepared as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention compds. have pIC50 values of ≥ 5 in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepared in four steps from 4-phenyl-4-piperidinecarbonitrile by protection of the piperidine with Boc anhydride, reduction of the nitrile with diisobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepared in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduction of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxymethylborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II.

ACCESSION NUMBER: 2004:534173 CAPLUS

DOCUMENT NUMBER: 141:89016

TITLE: Preparation of

benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection
INVENTOR(S): Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph; Bifulco, Neil; Boros, Eric Eugene; Chauder, Brian Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; Mclean, Ed Williams; Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin; Vanderwall, Dana

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; et al.; et al.

SOURCE: PCT Int. Appl., 859 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004054974	A2	20040701	WO 2003-US39644	20031212
WO 2004054974	A3	20040902		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,			

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
 NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
 TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
 TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2509711	A1	20040701	CA 2003-2509711	20031212
AU 2003300902	A1	20040709	AU 2003-300902	20031212
EP 1569646	A2	20050907	EP 2003-813419	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017230	A	20051025	BR 2003-17230	20031212
CN 1744899	A	20060308	CN 2003-80109628	20031212
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US 20060229336	A1	20061012	US 2005-538144	20050609
MX 2005006354	A	20050826	MX 2005-6354	20050613
IN 2005KN01328	A	20060630	IN 2005-KN1328	20050711
ZA 2005005600	A	20060927	ZA 2005-5600	20050712
PRIORITY APPLN. INFO.:			US 2002-433634P	P 20021213
			WO 2003-US39644	W 20031212
OTHER SOURCE(S):		MARPAT 141:89016		
REFERENCE COUNT:		11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT		

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